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Software Uncertainty in Integrated Environmental Modelling: the role of Semantics and Open Science

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Computational aspects increasingly shape environmental sciences [1]. Actually, transdisciplinary modelling of complex and uncertain environmental systems is challenging computational science (CS) and also the science-policy interface [2–7]. Large spatial-scale problems falling within this category – i.e. wide-scale transdisciplinary modelling for environment (WSTMe) [8–10] – often deal with factors **(a)** for which deep-uncertainty [2,7,11,12] may prevent usual statistical analysis of modelled quantities and need different ways for providing policy-making with science-based support.

Here, practical recommendations are proposed for tempering a peculiar – not infrequently underestimated – source of uncertainty. Software errors in complex WSTMe may subtly affect the outcomes with possible consequences even on collective environmental decision-making. Semantic transparency in CS [2,8,10,13,14] and free software [15,16] are discussed as possible mitigations **(b)**.

$$\begin{aligned}
 & \text{Complexity} = \left\{ \begin{array}{l} \text{Transdisciplinary integration (e.g. systems of systems)} \\ \text{Environmental system(s) heterogeneity (e.g. geospatial fragmentation)} \\ \text{Data heterogeneity (formats, definitions, spatiotemporal density, ...)} \\ \text{Software complexity (algorithms, dependencies, languages, interfaces, ...)} \end{array} \right. \\
 \\
 \text{(a)} \quad & \text{Uncertainty} = \left\{ \begin{array}{l} \text{Incomplete scientific knowledge} \\ \quad \text{(e.g. climate scenarios [17–19], tipping points [20–23], ...)} \\ \text{Modelling assumptions and simplifications [24–26]} \\ \text{Uncertainty of measured/derived data} \\ \text{Software uncertainty} \end{array} \right. \\
 \\
 & \text{Dynamic behaviour} = \left\{ \begin{array}{l} \text{Uncertainty propagation via:} \\ \quad \text{Propagation in the network of interconnected WSTMe components [2,14,27–33]} \\ \quad \text{Iterations within nonlinear optimization steps [5,34–40]} \\ \quad \text{Data fusion, harmonization, integration [9,41–44]} \\ \quad \text{Steps for computing and aggregating criteria and indices [6,7,11,12,45–48]} \end{array} \right.
 \end{aligned}$$

Software uncertainty, black-boxes and free software

Integrated natural resources modelling and management (INRMM) [28] frequently exploits chains of nontrivial data-transformation models (D-TM), each of them affected by uncertainties and errors. Those D-TM chains may be packaged as monolithic specialized models, maybe only accessible as black-box executables (if accessible at all) [49]. For end-users, black-boxes merely transform inputs in the final outputs, relying on classical peer-reviewed publications for describing the internal mechanism. While software tautologically plays a vital role in CS, it is often neglected in favour of more theoretical aspects. This paradox has been provocatively described as “the invisibility of software in published science. Almost all published papers required some coding, but almost none mention software, let alone include or link to source code” [50].

Recently, this primacy of theory over reality [51–53] has been challenged by new emerging hybrid approaches [54] and by the growing debate on open science and scientific knowledge freedom [2,55–58]. In particular, the role of free software has been underlined within the paradigm of reproducible research [49,57–59]. In the spectrum of reproducibility, the free availability of the source code is emphasized [57] as the first step from non-reproducible research (only based on classic peer-reviewed publications) toward reproducibility. Applying this paradigm to WSTMe, an alternative strategy to black-boxes would suggest exposing not only final outputs but also key intermediate layers of data and information along with the corresponding free software D-TM modules. A concise, semantically-enhanced modularization [13,14] may help not only to see the code (as a very basic prerequisite for semantic transparency) but also to understand – and correct – it [60]. Semantically-enhanced, concise modularization is e.g. supported by semantic array programming (SemAP) [13,14] and its extension to geospatial problems [8,10]. Some WSTMe may surely be classified in the subset of software systems which “are growing well past the ability of a small group of people to completely understand the content”, while “data from these systems are often used for critical decision making” [51]. In this context, the further uncertainty arising from the unpredicted “(not to say unpredictable)” [52] behaviour of software errors propagation in WSTMe should be explicitly considered as software uncertainty [61,62].

$Y = f^*(X) = f(\theta^*, X)$ Theoretic D-TM whose algorithm is typically described in peer reviewed publications. The D-TM may e.g. implement a given WSTMe as instance of a suitable family of functions f by means of selected parameters θ^* . θ^* may be the result of an optimization (regression, control problem, ...).

$Y = f^\zeta(X) = f(\theta^\zeta, X, \zeta)$ Real D-TM where the software uncertainty ζ may affect both the function family f and the optimality of the selected parameters θ^ζ .

$::| f(\theta, X, \zeta) |::^{sem}$ Semantically enhanced D-TM (e.g. SemAP). The D-TM is subject to the semantic checks *sem* as pre-, post-conditions and invariants on inputs, outputs and the D-TM itself:

$$Y = ::| f(\theta, X, \zeta) |::^{sem} \Leftrightarrow \begin{cases} Y = f(\theta, X, \zeta) \\ \square_{sem}(Y, f, \theta, X, \zeta) \end{cases}$$

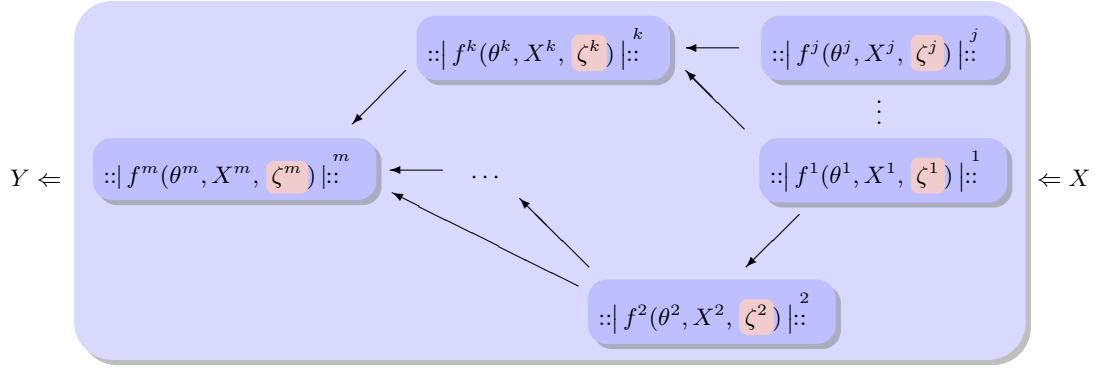
(b)

where $\begin{cases} X \text{ is the input array of data } X = \{X_1, X_2, \dots, X_i \dots X_n\} \\ X_i \in \mathbf{C}^{N_{i1} \times \dots \times N_{in_i}} \text{ is a multi-dimensional array (e.g. a two-dimensional raster layer)} \\ Y \text{ is analogously the output array of data} \\ \text{the modal/deontic logic operator } \square p \text{ means: it ought to be that } p. \end{cases}$

The data and information flow of a black-box D-TM is often a (hidden) composition of D-TM modules:

$$Y \Leftarrow \text{sem} \left[f(\theta, X, \zeta) \right] \Leftarrow X$$

This chain of free-software D-TM modules (each of them semantically-enhanced) should be transparent:



Semantics and design diversity

Silent faults [63] are a critical class of software errors altering computation output without evident symptoms – such as computation premature interruption (exceptions, error messages, ...), obviously unrealistic results or computation patterns (e.g. noticeably shorter/longer or endless computations). As it has been underlined, “many scientific results are corrupted, perhaps fatally so, by undiscovered mistakes in the software used to calculate and present those results” [64]. Despite the ubiquity of software errors [61–69], the structural role of scientific software uncertainty seems dramatically underestimated [2,52]. Semantic D-TM modularization might help to catch at least a subset of silent faults, when misusing intermediate data outside the expected semantic context of a given D-TM module (b).

Where the complexity and scale of WSTMe may lead unavoidable software-uncertainty to induce or worsen deep-uncertainty [2], techniques such as ensemble modelling may be recommendable [7,11,12]. Adapting those techniques for glancing at the software-uncertainty of a given WSTMe would imply availability of multiple instances (implementations) of the same abstract WSTMe. Independently re-implementing the same WSTMe (design diversity [70]) might of course be extremely expensive. However, partly independent re-implementations of critical D-TM modules may be more affordable and examples of comparison between supposedly equivalent D-TM algorithms seem to corroborate the interest of this research option [58,71,50].

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